

# Full wwPDB X-ray Structure Validation Report (i)

#### Oct 23, 2021 – 08:53 AM EDT

:	1JDA
:	MALTOTETRAOSE-FORMING EXO-AMYLASE
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:	1997-06-16
:	2.20  Å(reported)
	: : : :

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\# {\rm Entries,\ resolution\ range}({\rm \AA})) \end{array}$	
Clashscore	141614	5594 (2.20-2.20)	
Ramachandran outliers	138981	5503 (2.20-2.20)	
Sidechain outliers	138945	5504 (2.20-2.20)	

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain					
1	Δ	490						
	A	429	55%	31%	8% • •			



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3502 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called 1,4-ALPHA MALTOTETRAHYDROLASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	418	Total 3297	C 2070	N 597	O 620	S 10	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	219	GLN	GLU	engineered mutation	UNP P13507
А	334	ASP	SER	conflict	UNP P13507

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Ca 2 2	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	203	Total         O           203         203	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: 1,4-ALPHA MALTOTETRAHYDROLASE



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	65.70Å 171.00Å 46.80Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution(A)	10.00 - 2.20	Depositor
Resolution (A)	32.26 - 2.20	EDS
% Data completeness	(Not available) $(10.00-2.20)$	Depositor
(in resolution range)	96.0 (32.26-2.20)	EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.77 (at 2.20 \text{\AA})$	Xtriage
Refinement program	PROFFT, X-PLOR	Depositor
B B.	0.174 , (Not available)	Depositor
$\Lambda, \Lambda_{free}$	0.224 , (Not available)	DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	22.3	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31, 54.1	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.51, < L^2>=0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3502	wwPDB-VP
Average B, all atoms $(Å^2)$	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.85% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

# 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bo	nd lengths	Bond angles		
		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	1.14	3/3402~(0.1%)	2.25	104/4631~(2.2%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	А	248	ARG	CD-NE	-6.04	1.36	1.46
1	А	248	ARG	NE-CZ	-5.50	1.25	1.33
1	А	353	ARG	CZ-NH2	5.18	1.39	1.33

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	248	ARG	CD-NE-CZ	38.22	177.11	123.60
1	А	346	ARG	NE-CZ-NH1	25.66	133.13	120.30
1	А	196	ARG	NE-CZ-NH1	23.76	132.18	120.30
1	А	11	ARG	NE-CZ-NH1	23.76	132.18	120.30
1	А	248	ARG	NE-CZ-NH1	21.05	130.82	120.30
1	А	29	ARG	NE-CZ-NH1	20.92	130.76	120.30
1	А	29	ARG	CD-NE-CZ	19.30	150.62	123.60
1	А	358	ARG	NE-CZ-NH1	19.15	129.88	120.30
1	А	283	ARG	NE-CZ-NH2	-18.93	110.83	120.30
1	А	353	ARG	NE-CZ-NH1	16.91	128.76	120.30



Conti	Continued from previous page						
Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	283	ARG	NE-CZ-NH1	16.61	128.60	120.30
1	А	182	ARG	NE-CZ-NH2	-15.81	112.39	120.30
1	А	196	ARG	NE-CZ-NH2	-14.16	113.22	120.30
1	А	182	ARG	NE-CZ-NH1	13.19	126.89	120.30
1	А	146	TYR	CB-CA-C	12.81	136.02	110.40
1	А	82	ASP	CB-CG-OD1	-12.80	106.78	118.30
1	А	414	ARG	NE-CZ-NH2	-12.77	113.92	120.30
1	А	414	ARG	NE-CZ-NH1	12.22	126.41	120.30
1	А	34	ASP	CB-CG-OD1	12.21	129.29	118.30
1	А	61	ARG	NE-CZ-NH2	-11.57	114.52	120.30
1	А	175	ARG	NE-CZ-NH1	11.10	125.85	120.30
1	А	346	ARG	CD-NE-CZ	11.02	139.02	123.60
1	А	390	ASP	CB-CG-OD1	10.94	128.15	118.30
1	А	191	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	А	137	ARG	NE-CZ-NH1	10.23	125.42	120.30
1	А	353	ARG	CD-NE-CZ	9.95	137.53	123.60
1	А	146	TYR	CA-CB-CG	9.26	131.00	113.40
1	А	196	ARG	CD-NE-CZ	9.16	136.42	123.60
1	А	247	ASP	CB-CG-OD1	8.62	126.05	118.30
1	А	346	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	А	82	ASP	CB-CA-C	-8.39	93.61	110.40
1	А	194	PHE	C-N-CA	8.39	142.68	121.70
1	А	360	ASP	CB-CG-OD1	8.34	125.81	118.30
1	А	358	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	А	353	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	А	366	HIS	C-N-CA	8.17	142.12	121.70
1	А	338	ASP	CB-CG-OD2	8.13	125.62	118.30
1	А	248	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	А	242	ILE	CA-CB-CG2	8.11	127.11	110.90
1	А	346	ARG	NH1-CZ-NH2	-8.05	110.54	119.40
1	А	11	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	А	297	TYR	CB-CG-CD1	7.90	125.74	121.00
1	А	417	ARG	C-N-CA	7.76	141.10	121.70
1	А	255	ASP	CB-CG-OD2	7.72	125.25	118.30
1	А	416	TRP	C-N-CA	7.68	140.90	121.70
1	А	152	ASP	CB-CG-OD1	7.61	125.15	118.30
1	А	29	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	А	139	ASP	CB-CG-OD2	7.53	125.08	118.30
1	A	160	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	A	417	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	233	ARG	NE-CZ-NH1	-7.51	116.55	120.30
1	А	11	ARG	NH1-CZ-NH2	-7.44	111.22	119.40
1	1	1	1	1	1		1

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	137	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	А	390	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	А	316	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	А	92	ASP	CB-CG-OD2	6.90	124.51	118.30
1	А	414	ARG	CD-NE-CZ	6.89	133.24	123.60
1	А	409	SER	N-CA-CB	6.62	120.43	110.50
1	А	324	THR	CA-CB-CG2	6.59	121.63	112.40
1	А	62	ASP	CB-CG-OD2	6.58	124.22	118.30
1	А	68	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	А	29	ARG	NH1-CZ-NH2	-6.40	112.36	119.40
1	А	1	ASP	CB-CG-OD1	-6.37	112.56	118.30
1	А	358	ARG	CD-NE-CZ	6.34	132.47	123.60
1	А	369	TYR	CA-CB-CG	-6.20	101.63	113.40
1	А	343	ASP	CB-CG-OD1	6.17	123.85	118.30
1	А	261	ARG	CD-NE-CZ	6.00	132.00	123.60
1	А	175	ARG	NH1-CZ-NH2	-5.96	112.84	119.40
1	А	86	ASN	C-N-CA	5.91	134.71	122.30
1	А	248	ARG	NH1-CZ-NH2	-5.91	112.90	119.40
1	А	334	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	А	98	ALA	CB-CA-C	5.85	118.88	110.10
1	А	96	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	А	139	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	А	269	ASP	CB-CG-OD1	-5.77	113.11	118.30
1	А	242	ILE	CB-CA-C	5.72	123.04	111.60
1	А	175	ARG	CD-NE-CZ	5.70	131.57	123.60
1	А	96	ARG	CD-NE-CZ	-5.67	115.66	123.60
1	А	297	TYR	CB-CG-CD2	-5.66	117.61	121.00
1	А	372	LEU	CA-CB-CG	5.62	128.24	115.30
1	А	226	GLU	OE1-CD-OE2	5.62	130.05	123.30
1	A	181	LEU	CB-CA-C	5.62	120.87	110.20
1	A	142	ASP	CB-CG-OD1	-5.61	113.25	118.30
1	А	185	TYR	C-N-CA	5.61	134.08	122.30
1	A	45	THR	CA-CB-CG2	5.48	120.08	112.40
1	A	202	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	A	402	PHE	C-N-CA	5.46	135.34	121.70
1	A	338	ASP	O-C-N	5.44	131.40	122.70
1	А	319	TYR	CB-CG-CD1	-5.42	117.75	121.00
1	A	177	GLU	CG-CD-OE1	5.42	129.13	118.30
1	А	160	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	256	PHE	N-CA-CB	5.39	120.30	110.60
1	А	92	ASP	CB-CG-OD1	-5.26	113.56	118.30
1	А	195	VAL	CG1-CB-CG2	5.21	119.24	110.90



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	190	PHE	O-C-N	5.19	131.00	122.70
1	А	55	TRP	CA-CB-CG	5.10	123.40	113.70
1	А	291	ASP	N-CA-CB	5.09	119.76	110.60
1	А	181	LEU	N-CA-CB	-5.07	100.25	110.40
1	А	404	GLU	CA-CB-CG	5.07	124.55	113.40
1	А	341	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	А	36	TYR	CB-CG-CD1	5.06	124.04	121.00
1	А	109	VAL	CA-CB-CG1	5.04	118.47	110.90
1	А	251	CYS	CB-CA-C	-5.03	100.34	110.40
1	А	291	ASP	O-C-N	5.01	130.71	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	182	ARG	Sidechain
1	А	353	ARG	Sidechain

# 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3297	0	3011	145	0
2	А	2	0	0	0	0
3	А	203	0	0	12	0
All	All	3502	0	3011	145	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (145) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:SER:O	1:A:389:SER:HB2	1.24	1.24
1:A:71:LYS:HD3	1:A:302:ASN:OD1	1.61	1.01



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:277:ASN:HD22	1:A:279:ASP:H	1.07	1.01
1:A:370:SER:O	1:A:389:SER:CB	2.10	0.99
1:A:145:ASN:HD21	1:A:154:ASP:HB3	1.24	0.98
1:A:116:ASN:HD22	1:A:117:HIS:HD2	1.06	0.98
1:A:334:ASP:OD1	1:A:338:ASP:OD2	1.87	0.92
1:A:11:ARG:HH22	1:A:204:ASN:ND2	1.68	0.92
1:A:11:ARG:HH12	1:A:204:ASN:HD22	0.92	0.91
1:A:299:PRO:HD3	1:A:334:ASP:OD2	1.70	0.91
1:A:11:ARG:HH12	1:A:204:ASN:ND2	1.68	0.90
1:A:86:ASN:C	1:A:86:ASN:OD1	2.11	0.89
1:A:17:GLU:OE2	1:A:108:LYS:HE2	1.74	0.87
1:A:11:ARG:NH1	1:A:204:ASN:HD22	1.70	0.87
1:A:26:ASN:HD22	1:A:29:ARG:HH11	1.26	0.82
1:A:61:ARG:HD2	1:A:84:ASN:HB3	1.60	0.82
1:A:70:SER:O	1:A:71:LYS:HB2	1.79	0.79
1:A:116:ASN:HD22	1:A:117:HIS:CD2	1.96	0.79
1:A:277:ASN:ND2	1:A:279:ASP:H	1.79	0.79
1:A:211:ALA:HB1	1:A:214:SER:OG	1.83	0.78
1:A:143:PRO:HB2	1:A:146:TYR:HE1	1.48	0.78
1:A:409:SER:O	1:A:412:GLN:HG3	1.84	0.78
1:A:132:GLY:O	1:A:133:GLN:HG2	1.84	0.77
1:A:160:ASP:OD1	1:A:160:ASP:N	2.14	0.77
1:A:317:GLN:H	1:A:317:GLN:HE21	1.31	0.76
1:A:145:ASN:HD21	1:A:154:ASP:CB	2.01	0.73
1:A:61:ARG:NH1	1:A:82:ASP:OD2	2.21	0.73
1:A:86:ASN:OD1	1:A:87:GLY:N	2.22	0.73
1:A:216:CYS:O	1:A:252:PRO:HD2	1.88	0.73
1:A:319:TYR:OH	1:A:335:HIS:CD2	2.42	0.73
1:A:24:HIS:HD2	1:A:26:ASN:H	1.38	0.72
1:A:292:ASN:ND2	1:A:294:ASP:H	1.89	0.70
1:A:358:ARG:HG3	3:A:530:HOH:O	1.91	0.69
1:A:82:ASP:HB3	1:A:84:ASN:H	1.60	0.67
1:A:24:HIS:HE1	3:A:489:HOH:O	1.77	0.66
1:A:11:ARG:NH2	1:A:204:ASN:ND2	2.41	0.65
1:A:85:LYS:NZ	1:A:177:GLU:OE2	2.26	0.65
1:A:292:ASN:ND2	1:A:295:THR:H	1.94	0.65
1:A:154:ASP:OD2	1:A:196:ARG:HD3	1.97	0.65
1:A:145:ASN:ND2	1:A:155:ARG:H	1.94	0.65
1:A:277:ASN:HD22	1:A:279:ASP:N	1.87	0.65
1:A:71:LYS:CD	1:A:302:ASN:OD1	2.43	0.64
1:A:61:ARG:HD3	1:A:82:ASP:HB2	1.78	0.64



	A the C	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:388:ASN:ND2	1:A:412:GLN:HB3	2.12	0.64
1:A:407:ASN:C	1:A:407:ASN:HD22	2.02	0.62
1:A:3:ALA:HB2	1:A:13:HIS:CE1	2.34	0.62
1:A:143:PRO:HD2	3:A:578:HOH:O	1.99	0.62
1:A:84:ASN:OD1	1:A:86:ASN:HB3	2.01	0.61
1:A:332:TYR:HB3	1:A:335:HIS:CD2	2.35	0.61
1:A:402:PHE:CD1	1:A:417:ARG:HB2	2.35	0.61
1:A:319:TYR:OH	1:A:335:HIS:HD2	1.83	0.61
1:A:88:ARG:HB2	3:A:662:HOH:O	2.01	0.61
1:A:11:ARG:HH22	1:A:204:ASN:HD21	1.46	0.60
1:A:144:GLY:O	1:A:146:TYR:N	2.32	0.60
1:A:258:LEU:HB2	1:A:273:GLY:HA3	1.84	0.60
1:A:42:GLN:HG3	3:A:597:HOH:O	2.02	0.59
1:A:3:ALA:HB1	1:A:13:HIS:NE2	2.18	0.59
1:A:3:ALA:CB	1:A:13:HIS:CE1	2.86	0.59
1:A:167:HIS:HD2	1:A:169:GLN:H	1.49	0.58
1:A:38:ILE:O	1:A:42:GLN:HG2	2.03	0.58
1:A:332:TYR:HB3	1:A:335:HIS:HD2	1.69	0.57
1:A:61:ARG:CD	1:A:84:ASN:HB3	2.31	0.57
1:A:182:ARG:HD2	1:A:211:ALA:HB2	1.85	0.57
1:A:116:ASN:ND2	1:A:117:HIS:HD2	1.90	0.56
1:A:325:SER:HB2	1:A:326:PRO:CD	2.36	0.56
1:A:299:PRO:CD	1:A:334:ASP:OD2	2.51	0.55
1:A:312:ASP:HA	1:A:315:ILE:HG13	1.88	0.55
1:A:292:ASN:HD21	1:A:294:ASP:HB2	1.71	0.55
1:A:292:ASN:HD22	1:A:294:ASP:H	1.54	0.55
1:A:19:ILE:HD13	1:A:328:THR:CG2	2.38	0.54
1:A:61:ARG:HB3	1:A:84:ASN:O	2.08	0.54
1:A:321:TYR:HB2	1:A:387:LEU:HD11	1.90	0.54
1:A:402:PHE:HD1	1:A:417:ARG:HB2	1.73	0.54
1:A:122:TYR:CD1	1:A:123:PRO:HD2	2.43	0.53
1:A:87:GLY:O	1:A:88:ARG:HB2	2.09	0.53
1:A:335:HIS:HE1	3:A:522:HOH:O	1.92	0.53
1:A:333:TRP:HD1	1:A:334:ASP:OD1	1.92	0.53
1:A:88:ARG:NH1	3:A:564:HOH:O	2.41	0.53
1:A:355:ALA:CB	1:A:381:GLN:HB2	2.39	0.53
1:A:167:HIS:CD2	1:A:169:GLN:HB3	2.43	0.53
1:A:404:GLU:OE1	1:A:407:ASN:HB2	2.09	0.53
1:A:191:ARG:NH1	1:A:193:ASP:HB2	2.23	0.52
1:A:11:ARG:NH1	1:A:204:ASN:ND2	2.42	0.52
1:A:114:VAL:O	1:A:114:VAL:HG12	2.08	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:43:ALA:HB2	1:A:102:LEU:HD13	1.91	0.52
1:A:303:GLY:HA2	3:A:562:HOH:O	2.10	0.52
1:A:323:LEU:O	1:A:352:ARG:HD2	2.10	0.52
1:A:390:ASP:O	1:A:391:LEU:C	2.48	0.51
1:A:122:TYR:CG	1:A:123:PRO:HD2	2.46	0.51
1:A:244:ASP:O	1:A:248:ARG:HG3	2.10	0.51
1:A:26:ASN:ND2	1:A:29:ARG:HH11	2.01	0.51
1:A:2:GLN:O	1:A:14:GLY:HA3	2.10	0.51
1:A:220:LEU:HD23	1:A:242:ILE:HD12	1.92	0.51
1:A:29:ARG:NH2	1:A:76:GLU:OE2	2.24	0.50
1:A:61:ARG:HD3	1:A:82:ASP:CB	2.42	0.50
1:A:366:HIS:HB2	1:A:373:VAL:HG22	1.92	0.50
1:A:143:PRO:HB2	1:A:146:TYR:CE1	2.38	0.50
1:A:195:VAL:CG1	1:A:220:LEU:HB2	2.41	0.50
1:A:81:HIS:HD2	3:A:495:HOH:O	1.94	0.50
1:A:279:ASP:OD1	1:A:280:PRO:HD2	2.11	0.50
1:A:200:PRO:HB2	1:A:248:ARG:HB2	1.94	0.49
1:A:319:TYR:O	1:A:323:LEU:HB2	2.12	0.49
1:A:320:ALA:HA	1:A:348:LEU:HD13	1.95	0.49
1:A:137:ARG:NH2	1:A:146:TYR:O	2.33	0.48
1:A:167:HIS:CD2	1:A:169:GLN:H	2.30	0.48
1:A:19:ILE:HD13	1:A:328:THR:HG22	1.95	0.48
1:A:43:ALA:CB	1:A:102:LEU:HD13	2.44	0.48
1:A:373:VAL:HA	1:A:385:VAL:O	2.13	0.48
1:A:195:VAL:HG11	1:A:220:LEU:HB2	1.96	0.47
1:A:115:PRO:HG2	1:A:198:TYR:CZ	2.49	0.46
1:A:417:ARG:CG	3:A:544:HOH:O	2.63	0.46
1:A:111:TYR:CD2	1:A:187:ALA:HB2	2.50	0.46
1:A:202:ARG:O	1:A:205:SER:HB2	2.16	0.46
1:A:325:SER:HB2	1:A:326:PRO:HD2	1.99	0.45
1:A:145:ASN:ND2	1:A:154:ASP:HB3	2.09	0.45
1:A:382:THR:O	1:A:417:ARG:HB3	2.17	0.45
1:A:292:ASN:HD22	1:A:294:ASP:N	2.13	0.45
1:A:42:GLN:CG	3:A:597:HOH:O	2.63	0.45
1:A:145:ASN:HD21	1:A:155:ARG:H	1.65	0.44
1:A:323:LEU:HD12	1:A:323:LEU:HA	1.88	0.44
1:A:1:ASP:OD2	1:A:108:LYS:NZ	2.51	0.44
1:A:60:TRP:HB3	1:A:82:ASP:O	2.18	0.44
1:A:387:LEU:O	1:A:388:ASN:C	2.56	0.44
1:A:292:ASN:HD22	1:A:292:ASN:C	2.22	0.44
1:A:115:PRO:HG2	1:A:198:TYR:CE2	2.53	0.43



A + am 1	A + 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:292:ASN:ND2	1:A:294:ASP:N	2.62	0.43
1:A:261:ARG:NE	1:A:261:ARG:HA	2.32	0.43
1:A:344:PHE:CZ	1:A:348:LEU:HD11	2.53	0.43
1:A:194:PHE:CD2	1:A:194:PHE:O	2.72	0.43
1:A:182:ARG:HD2	1:A:211:ALA:CB	2.49	0.43
1:A:118:MET:O	1:A:161:ALA:HB1	2.20	0.42
1:A:191:ARG:HH11	1:A:193:ASP:HB2	1.85	0.42
1:A:35:TRP:CE3	1:A:38:ILE:HD12	2.54	0.42
1:A:96:ARG:HH11	1:A:96:ARG:HD3	1.66	0.42
1:A:66:TRP:CE3	1:A:66:TRP:O	2.73	0.42
1:A:78:TYR:O	1:A:117:HIS:HE1	2.02	0.42
1:A:372:LEU:HA	3:A:480:HOH:O	2.21	0.41
1:A:3:ALA:HB1	1:A:13:HIS:CE1	2.55	0.41
1:A:69:GLY:O	1:A:70:SER:C	2.58	0.41
1:A:11:ARG:NH2	1:A:204:ASN:HD21	2.14	0.41
1:A:237:SER:H	1:A:240:GLN:HE21	1.68	0.41
1:A:409:SER:O	1:A:412:GLN:CG	2.63	0.40
1:A:150:CYS:O	1:A:164:ASN:HB2	2.22	0.40
1:A:282:TRP:O	1:A:285:VAL:HG22	2.22	0.40
1:A:306:HIS:O	1:A:306:HIS:ND1	2.54	0.40

There are no symmetry-related clashes.

# 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	416/429~(97%)	386~(93%)	21 (5%)	9~(2%)	6 4

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	70	SER
	~		



Conti	Continueu from previous page					
Mol	Chain	Res	Type			
1	А	71	LYS			
1	А	87	GLY			
1	А	133	GLN			
1	А	68	ASP			
1	А	123	PRO			
1	А	132	GLY			
1	А	301	GLN			
1	А	157	ILE			

#### 5.3.2Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	333/337~(99%)	296~(89%)	37 (11%)	6 5

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	12	TYR
1	А	19	ILE
1	А	55	TRP
1	А	61	ARG
1	А	68	ASP
1	А	71	LYS
1	А	79	PHE
1	А	86	ASN
1	А	95	LEU
1	А	102	LEU
1	А	109	VAL
1	А	119	ASN
1	А	125	LYS
1	А	146	TYR
1	А	157	ILE
1	А	160	ASP
1	А	162	ASP
1	А	195	VAL



Mol	Chain	Res	Type
1	А	196	ARG
1	А	248	ARG
1	А	290	VAL
1	А	292	ASN
1	А	308	TRP
1	А	317	GLN
1	А	323	LEU
1	А	353	ARG
1	А	358	ARG
1	А	364	SER
1	А	367	SER
1	А	373	VAL
1	А	383	LEU
1	А	389	SER
1	А	397	VAL
1	А	404	GLU
1	А	407	ASN
1	А	409	SER
1	А	418	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	2	GLN
1	А	24	HIS
1	А	26	ASN
1	А	81	HIS
1	А	97	GLN
1	А	117	HIS
1	А	119	ASN
1	А	145	ASN
1	А	167	HIS
1	А	180	ASN
1	А	204	ASN
1	А	240	GLN
1	А	264	ASN
1	А	277	ASN
1	А	292	ASN
1	А	317	GLN
1	А	335	HIS
1	А	366	HIS
1	А	388	ASN



Continued from previous page...

Mol	Chain	$\operatorname{Res}$	Type
1	А	407	ASN

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

# 5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

# 5.7 Other polymers (i)

There are no such residues in this entry.

# 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

# 6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

# 6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

# 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

# 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

# 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

